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Maximising the permanent and complementary permanent of (0,1)-matrices with constant line sum

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Abstract

Let Λ_n^k denote the set of $(0,1)$-matrices of order n with exactly k ones in each row and column. Let J_i be such that $\Lambda_i^i = \{J_i\}$ and for $A \in \Lambda_n^k$ define $\overline{A} \in \Lambda_n^{n-k}$ by $\overline{A} = J_n - A$. We are interested in the matrices in Λ_n^k which maximise the permanent function. Consider the sets

$$M_n^k = \{A \in \Lambda_n^k\colon \ \mathrm{per}(A) \geqslant \mathrm{per}(B), \ \text{for all } B \in \Lambda_n^k\},$$
$$\overline{M}_n^k = \{A \in \Lambda_n^k\colon \ \mathrm{per}(\overline{A}) \geqslant \mathrm{per}(\overline{B}), \ \text{for all } B \in \Lambda_n^k\}.$$

For k fixed and n sufficiently large we prove the following results.

1. Modulo permutations of the rows and columns, every member of $M_n^k \cup \overline{M}_n^k$ is a direct sum of matrices of bounded size of which fewer than k differ from J_k.
2. $A \in M_n^k$ if and only if $A \oplus J_k \in M_{n+k}^k$.
3. $A \in \overline{M}_n^k$ if and only if $A \oplus J_k \in \overline{M}_{n+k}^k$.
4. $M_n^3 = \overline{M}_n^3$ if $n \equiv 0$ or $1 \pmod 3$ but $M_n^3 \cap \overline{M}_n^3 = \emptyset$ if $n \equiv 2 \pmod 3$.

We also conjecture the exact composition of $\overline{M}_n^k$ for large n, which is equivalent to identifying regular bipartite graphs with the maximum number of 4-cycles.

Keywords: Permanent; $(0,1)$-matrices; Rook polynomials; Regular bipartite graphs

1. Background

We use Λ_n^k to denote the set of $(0,1)$-matrices of order n which have exactly k ones in each row and column. The *permanent* function on Λ_n^k is defined by

$$\mathrm{per}(A) = \sum_{\tau} \prod_{i=1}^{n} A_{i,\tau(i)},$$

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where the sum is over all permutations τ in the symmetry group on n objects. The *subpermanent sum* $\sigma_i(A)$ is the sum of the permanents of all the order i submatrices of A. We adopt the convention that $\sigma_0(A)=1$.

Let I_n be the order n identity, J_n the order n matrix in which every entry is 1, and P_n the permutation matrix corresponding to the full cycle permutation $(123\cdots n)$. We define the *complement* of a matrix $A\in\Lambda_n^k$ by $\overline{A}=J_n-A\in\Lambda_n^{n-k}$. Let $D_n=\overline{I_n}$. We use $\oplus$ to denote the direct sum operator, and use rA as shorthand for $A\oplus A\oplus\cdots\oplus A$ (where there are r copies of A). We trust that this notation will not mislead; there being no call for scalar multiplication of matrices in this paper.

With $A\in\Lambda_n^k$ we associate a bipartite graph $G(A)$ where the two vertex sets correspond to the rows and columns respectively of A, and the edges of $G(A)$ correspond to the positive entries in A. Note that $G(A)$ is a k-regular spanning subgraph of the complete bipartite graph $K_{n,n}$. The permanent of A is the number of perfect matchings in $G(A)$. More generally, $\sigma_i(A)$ is the number of i-matchings in $G(A)$.

We find it useful to apply graph theoretic terminology to our matrices. For example, we say that $A,B\in\Lambda_n^k$ are isomorphic (written $A\cong B$) when we really mean that $G(A)$ and $G(B)$ are isomorphic. Since the permanent function is invariant over isomorphic matrices we are only interested in the structure of any matrix up to isomorphism. We also refer to the components of a matrix. If $A\cong C_1\oplus C_2\oplus\cdots\oplus C_a$ where each C_i is fully indecomposable, then we say that the C_i are the components of A. Of course the connected components of $G(A)$ in this case are $G(C_1),G(C_2),\ldots,G(C_a)$. Note that when we refer to the order of a component C_i, denoted by $\operatorname{ord}(C_i)$, we mean the order of the matrix C_i not the order of $G(C_i)$, which is $2\operatorname{ord}(C_i)$.

We are interested in identifying the matrices A in Λ_n^k which maximise $\operatorname{per}(A)$, and also those which maximise $\operatorname{per}(\overline{A})$. Note that since $\overline{A}\in\Lambda_n^{n-k}$ we are essentially asking the same question twice. However, we still find this a constructive approach. Formally, we define

$$M_n^k=\{A\in\Lambda_n^k:\ \operatorname{per}(A)\geqslant\operatorname{per}(B),\ \text{for all } B\in\Lambda_n^k\},$$

$$\overline{M}_n^k=\{A\in\Lambda_n^k:\ \operatorname{per}(\overline{A})\geqslant\operatorname{per}(\overline{B}),\ \text{for all } B\in\Lambda_n^k\}.$$

Our aim is to investigate elements of the two sets above; which turn out to have a number of common features. Our answers will involve the function $s(A)$, being the number of 4-cycles in $G(A)$ and S_n^k, the subset of matrices which maximise $s(\cdot)$ in Λ_n^k.

The problem was partly solved by Brègman [2] who showed that if A is a $(0,1)$-matrix of order n with column sums $c_1,c_2,\ldots,c_n$, then

$$\operatorname{per}(A)\leqslant\prod_{i=1}^{n}(c_i!)^{1/c_i}. \tag{1}$$

Moreover equality holds in (1) if and only if $A\cong mJ_k\in\Lambda_n^k$ for some integers k, m and $n=mk$. More recently, in [6] it was proved that if $n=mk$ for $m\geqslant5$ then $\overline{M}_n^k$

consists of those A for which $A \cong mJ_k$. Hence $\overline{M}_n^k = M_n^k$ in this instance; raising the question of whether the two sets are equal under more general conditions. Interestingly, it was also shown in [6] that $\overline{M}_6^2 \cap M_6^2 = \emptyset$ and $\overline{M}_9^3 \cap M_9^3 = \emptyset$, meaning that the general pattern excludes some small cases. This paper extends these ideas to cases when n is not necessarily a multiple of k.

One of our tools is the rook polynomial $\rho(A)$ given by

$$\rho(A) = \rho(A,x) = \sum_{i=0}^{n} (-1)^i \sigma_i(A) x^{n-i}.$$

The following important property of the rook polynomial is given by Godsil [4]. For any $A \in \Lambda_n^k$,

$$\mathrm{per}(\overline{A}) = \int_0^\infty \rho(A) \mathrm{e}^{-x} \, \mathrm{d}x. \tag{2}$$

We note two other properties of the rook polynomial. Firstly, it is multiplicative on components. That is, if $\{C_i\}_i$ is the set of components of A then $\rho(A) = \prod_i \rho(C_i)$. Secondly, for each positive integer a,

$$\rho(J_a) = \mathscr{L}_a(x) = (-1)^a a! \sum_{i=0}^{a} \binom{a}{i} \frac{(-x)^i}{i!}. \tag{3}$$

Note that $\mathscr{L}_a(x)$ is a Laguerre polynomial, normalised to be monic. It is intimately involved with the theory of rook polynomials, as demonstrated by the following result from [4],

$$\rho(\overline{A}) = \sum_{i=0}^{n} \sigma_{n-i}(A) \mathscr{L}_i(x). \tag{4}$$

Another result we need comes from [5], where it was proved in the context of extensions to Latin rectangles. For fixed k,

$$\mathrm{per}(\overline{A}) = n!(1 - k/n)^n \exp\left(\frac{k}{2n} + \frac{k(3k-1)}{n^2} + f + \frac{s(A)}{n^4} + \frac{(4k-2)s(A)}{n^5} + \mathrm{O}(n^{-5}) \right), \tag{5}$$

uniformly over $A \in \Lambda_n^k$, as $n \to \infty$. The function f is specified in [5], but we only need to know that it is independent of A and that $f = \mathrm{O}(n^{-3})$.

In the next section we prove a number of results about M_n^k and $\overline{M}_n^k$, often finding similarities between the two sets. In Section 3 we pose some conjectures regarding the exact composition of $\overline{M}_n^k$ for $n \gg k$. We follow with a section containing specific examples for small k. In the final section we examine the ramifications of our results for previously posed problems from [6,8].

2. The results

Our first goal is to show that components of matrices in M_n^k or $\overline{M_n}^k$ cannot be arbitrarily large. We begin by proving a technical lemma, involving the functions

$$\begin{aligned} &F(a,b)=(a!)^{b/a},\\ &D(k)=F(k,1)/F(k-1,1),\\ &C(k)=D(k)/D(k-1),\\ &B(k,v)=C(k)^v((k-v)^2+2v(k-v)D(k-1)+v(v-1)(D(k-1))^2). \end{aligned} \tag{6}$$

Lemma 1. *For every integer $k\geqslant 3$ there exists $\varepsilon_k>0$ such that $B(k,v)<k^2-\varepsilon_k$ for each integer v satisfying $0<v<k$.*

Proof. We start by showing that $D(k)$ is a decreasing function of k (interpolating factorials by using the gamma function). Note,

$$\frac{\mathrm{d}}{\mathrm{d}k}\log D(k)=\frac{2k-1}{k^2(k-1)^2}\log(k!)+\frac{1-\psi(k+1)}{k(k-1)}-\frac{\log k}{(k-1)^2},$$

where $\psi(k+1)=\frac{\mathrm{d}}{\mathrm{d}k}\log(k!)\geqslant\log k$. Now by 6.1.42 of [1],

$$(k+\tfrac{1}{2})\log k-k+\tfrac{1}{2}\log(2\pi)\leqslant\log(k!)\leqslant(k+\tfrac{1}{2})\log k-k+1 \tag{7}$$

for $k\geqslant 2$. Hence for $k\geqslant 3$,

$$\frac{\mathrm{d}}{\mathrm{d}k}\log D(k)\leqslant-\frac{(2k-1)(2k-2\log k-3)+1}{k^2(k-1)^2}<0.$$

It follows that $D(k)$ is a decreasing function, that $D(k)>\lim_{x\to\infty}D(x)=1$ and that $0<C(k)<1$ for $k\geqslant 4$.

Next we consider $B(k,v)$ as a continuous function of v. Observe that $B(k,v)$ has a critical point in the interval $[0,k]$ because $B(k,0)=B(k,k)=k^2$. Also

$$\frac{\partial}{\partial v}B(k,v)=C(k)^v((\Delta\log C(k))v^2+(2\Delta-\Phi\log C(k))v-\Phi+k^2\log C(k)), \tag{8}$$

where $\Delta=(D(k-1)-1)^2$ and $\Phi=(D(k-1))^2-2kD(k-1)+2k$. We conclude that $\frac{\partial}{\partial v}B(k,v)$ has precisely two roots, and that they are placed symmetrically about

$$v=v_0=\frac{-1}{\log C(k)}+\frac{\Phi}{2\Delta}. \tag{9}$$

If we can show that $v_0>k$ then the lemma will follow from Eq. (8), since $0<C(k)<1$ implies that $\frac{\partial}{\partial v}B(k,v)$ is negative whenever $|v|$ is sufficiently large.

Considering Φ/Δ as a function of a single variable $D(k-1)\in(1,\infty)$ it is elementary to show that $\Phi/\Delta\geqslant-k(k-2)$. Also, by applying Eq. (7) to

$$\log C(k)=\frac{1}{k}\log k-\frac{1}{k-2}\log(k-1)+\frac{2}{k(k-1)(k-2)}\log(k-1)!$$

for $k \geqslant 3$ we get

$$k(k-1)(k-2)\log C(k) \geqslant (k^2-3k+1)\log\frac{k}{k-1} - 2k + 2 + \log(2\pi k)$$
$$> (k^2-3k+1)\frac{1}{k} - 2k + 3$$
$$> -k.$$

Hence Eq. (9) yields

$$v_0 > (k-1)(k-2) - \tfrac{1}{2}k(k-2) = \tfrac{1}{2}(k-2)^2.$$

Note that $\frac{1}{2}(k-2)^2 \geqslant k$ for all $k \geqslant 3+\sqrt{5} \approx 5.2$. The lemma can be checked by enumeration for $k=3,4$ and 5. $\square$

Theorem 1. *For each $A \in \Lambda_a^k$ there exists $m(A)$ such that $\mathrm{per}(A \oplus tJ_k) > \mathrm{per}(B)$ for every integer t such that $a + tk \geqslant m(A)$ and every $B \in \Lambda_{a+tk}^k$ which does not contain J_k as a component.*

Proof. The statement is vacuous when $k=1$. If $k=2$ it follows easily from the fact that $\mathrm{per}(A \oplus tJ_2) \geqslant 2^{t+1}$ whereas $\mathrm{per}(B) \leqslant 2^{(2t+a)/3}$. Henceforth we assume $k \geqslant 3$.

Suppose $B \in \Lambda_n^k$ does not contain J_k as a component. Let U be the vertex set of $G(B)$ corresponding to rows of B, and let d be the standard metric on $G(B)$. Choose $X = \{x_i\} \subset U$ such that $d(x_i, x_j) > 6$ for $i \neq j$. Note that we do not specify $|X|$. All that is important is that we can make $|X|$ arbitrarily large provided we choose our initial value of n large enough. This follows from the observation that the diameter of a k-regular connected component increases without bound as its order increases.

Next for each $x_i \in X$ we choose $y_i \in U$ so that y_i has a proper subset of its neighbours in common with x_i. This is always possible given that no x_i is in a complete component. Let v_i be the number of common neighbours of x_i and y_i. Note that $1 \leqslant v_i \leqslant k-1$. Also, by choice $d(x_i, y_i) = 2$ for all i and the neighbourhoods of $\{x_i, y_i\}$ and $\{x_j, y_j\}$ are disjoint provided $i \neq j$.

We consider a partial expansion of $\mathrm{per}(B)$ along the rows $x_1, y_1, x_2, y_2, x_3, y_3, \ldots,$ of B and use (1) to bound the unexpanded part (see Fig. 1); giving

$$\mathrm{per}(B) \leqslant F\left(k, n - \sum_i (2k - v_i)\right) \prod_i [(k-v_i)^2 F(k-1, 2k-2v_i-2) F(k-2, v_i)$$
$$+ 2v_i(k-v_i) F(k-1, 2k-2v_i-1) F(k-2, v_i-1)$$
$$+ v_i(v_i-1) F(k-1, 2k-2v_i) F(k-2, v_i-2)].$$

Hence

$$\mathrm{per}(B) \leqslant F(k,n) \prod_i \left[\frac{F(k-1, 2k-2)}{F(k, 2k)} \frac{F(k, v_i) F(k-2, v_i)}{F(k-1, 2v_i)}\right.$$
$$\left.\times \left[\left((k-v_i)^2 + 2v_i(k-v_i)\frac{F(k-1,1)}{F(k-2,1)} + v_i(v_i-1)\frac{F(k-1,2)}{F(k-2,2)}\right)\right]\right],$$

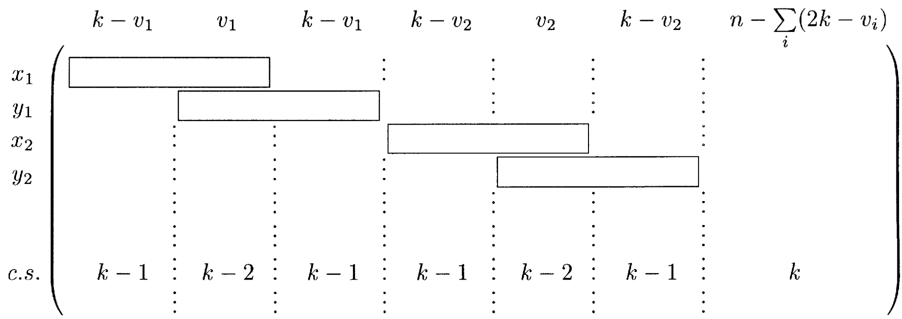

Fig. 1. Partial expansion of per(B). In this example $|X|=2$, and the rows and columns have (possibly) been permuted for the sake of convenience. We expand the permanent through the four rows: x_1, y_1, x_2 and y_2. The k positive entries in each of these rows are represented schematically by a box $\boxed{}$. The overlap structure of these boxes determines $7=3|X|+1$ distinct vertical *regions*. The number of columns in each region is listed above the matrix.

The rows below y_2 in our diagram collectively form the *unexpanded part*. Column sums (*c.s.*) in the unexpanded part are given for each region. Each term in our expansion of per(B) selects one entry from each box together with the permanent of the appropriate submatrix of the unexpanded part. We use Brègman's theorem (1) to bound this permanent. The bound depends only on the regions from which the entries in each box were selected.

which in the language of Eq. (6) simplifies to

$$\mathrm{per}(B)\leqslant F(k,n)\prod_i \frac{1}{k^2}B(k,v_i). \tag{10}$$

Now we apply Lemma 1 to see that we can make per(B) less than an arbitrarily small fraction of $F(k,n)$ by taking $|X|$ large enough.

By contrast, for $n=a+tk$,

$$\mathrm{per}(A\oplus tJ_k)=(k!)^t\mathrm{per}(A)=F(k,n)\mathrm{per}(A)/F(k,a).$$

Specifically per($A\oplus tJ_k$) remains a fixed fraction of $F(k,n)$ as t varies. We conclude that when t and hence n is sufficiently large, $\mathrm{per}(B)<\mathrm{per}(A\oplus tJ_k)$ as required. □

We next show the equivalent result to Theorem 1 for the case of complementary permanents. Note that for any matrices A, B and X the inequality $\mathrm{per}(A)>\mathrm{per}(B)$ implies $\mathrm{per}(A\oplus X)>\mathrm{per}(B\oplus X)$. However, from $\mathrm{per}(\overline{A})>\mathrm{per}(\overline{B})$ it does not necessarily follow that $\mathrm{per}(\overline{A\oplus X})>\mathrm{per}(\overline{B\oplus X})$. To deal with this obstacle we define a vacuous matrix V such that $A\oplus V=A$ for all A; and the set

$$\Upsilon_k=\{V\}\cup\Lambda_k^k\cup\Lambda_{k+1}^k\cup\Lambda_{k+2}^k\cup\cdots$$

Theorem 2. *For any $A\in\Lambda_n^k$ there exists $\overline{m}(A)$ such that* $\mathrm{per}(\overline{A\oplus tJ_k\oplus X})>\mathrm{per}(\overline{B\oplus X})$ *for every $X\in\Upsilon_k$ and t such that $n+tk\geqslant\overline{m}(A)$ and any $B\in\Lambda_{n+tk}^k$ which does not contain J_k as a component.*

Proof. Let k be fixed. For $A,B\in\Lambda_n^k$, where n is sufficiently large, we know from (5) that $\operatorname{per}(\overline{A}) > \operatorname{per}(\overline{B})$ whenever $s(A) > s(B)$. It follows that when n is large enough,

$$\overline{M}_n^k \subseteq S_n^k. \tag{11}$$

It is shown in [6] (and is easy to verify) that a vertex of a k-regular bipartite graph can be contained in at most $(k-1)\binom{k}{2}$ cycles of length 4. Moreover this bound is achieved uniquely when the vertex is in a complete component, $K_{k,k}$. Hence by taking t sufficiently large, the average number of 4-cycles incident with a vertex in $G(A\oplus tJ_k)$ can be made arbitrarily close to $(k-1)\binom{k}{2}$. By contrast, for any $B\in\Lambda_{n+tk}^k$ which does not contain J_k as a component, the average number of 4-cycles per vertex in $G(B)$ is certainly no more than $(k-1)\binom{k}{2}-1$. Thus when t is large enough $s(A\oplus tJ_k) > s(B)$. $\square$

Theorem 3. *For each integer k there exists b_k such that for any n and any $A\in M_n^k\cup\overline{M}_n^k$ the largest component in A is of order at most b_k.*

Proof. For each integer i in the interval $[k,2k)$ select any $A_i\in\Lambda_i^k$. Define b_k by

$$b_k=\max\{m(A_k),m(A_{k+1}),\ldots,m(A_{2k-1})\},$$

where $m(\cdot)$ is defined by Theorem 1. Now suppose that $A\in M_n^k$ contains a component C bigger than b_k. Since C is connected it does not contain a J_k. Hence Theorem 1 tells us that $\operatorname{per}(A)$ can be increased by substituting $A_i\oplus tJ_k$ for C, where $k\leqslant i\leqslant 2k-1$, $i\equiv \operatorname{ord}(C) \bmod k$ and $t=(\operatorname{ord}(C)-i)/k$. This contradicts A's membership of M_n^k. The above proof can now be repeated for $A\in\overline{M}_n^k$ using Theorem 2. $\square$

We define b_k^* to be the smallest integer having the property of b_k in Theorem 3. Note that $b_k^*\geqslant 2k-1$ because every element of M_{2k-1}^k consists of a single component. We now know that the size of components is bounded and hence the number of components grows with n. Our next goal is to characterise these components. But first, we prove another technical lemma.

Lemma 2. *For any $A\in\Lambda_n^k$ and $0\leqslant a<n$,*

$$\frac{\sigma_a(A)}{\sigma_{a+1}(A)}\geqslant\frac{a+1}{(n-a)^2}.$$

Proof. Each $(a+1)$-matching M in $G(A)$ can be converted to an a-matching by removing any one of the $a+1$ edges in M. By contrast, any a-matching M' can be extended to an $(a+1)$-matching in at most $(n-a)^2$ ways. This is because the subgraph induced by the vertices left uncovered by M' is isomorphic to a subgraph of $K_{n-a,n-a}$, and hence has no more than $(n-a)^2$ edges. The result follows. $\square$

For our next result we need a new definition. We define an ordering $\succ$ on Λ_n^k as follows. For $A, B \in \Lambda_n^k$ we say that $A \succ B$ if there exists j such that $\sigma_j(A) > \sigma_j(B)$ and $\sigma_i(A) = \sigma_i(B)$ for all $i < j$. We say that $A \in \Lambda_n^k$ is *$\succ$-maximal* if there does not exist $B \in \Lambda_n^k$ such that $B \succ A$.

Theorem 4. *For positive integers k and m there exists $N_{k,m} > 2m$ with the following property. If $A \cong C \oplus D \in \overline{M}_n^k$ where $n > N_{k,m}$ and* $\operatorname{ord}(C) \leqslant m$ *then $\overline{C}$ is $\succ$-maximal.*

Proof. Suppose $A \in \overline{M}_n^k$ and that $A \cong C \oplus D$ where $\operatorname{ord}(C) \leqslant m < \operatorname{ord}(D)$. Consider the rook polynomials $\rho(A) = \rho(C)\rho(D)$. We express $\rho(C)$ and $\rho(D)$ in the Laguerre basis, so that $\rho(C) = \sum c_i \mathscr{L}_i(x)$ and $\rho(D) = \sum d_i \mathscr{L}_i(x)$. Then

$$\operatorname{per}(\overline{A}) = \int_0^\infty \mathrm{e}^{-x} \rho(C)\rho(D)\,\mathrm{d}x = \sum_{i=1}^{\operatorname{ord}(C)} (i!)^2 c_i d_i \tag{12}$$

by Eq. (2) and the orthogonality of the Laguerre polynomials. Also by Eq. (4) we know that $d_i = \sigma_{\operatorname{ord}(D)-i}(\overline{D})$ so Lemma 2 applied for $i < \operatorname{ord}(C) \leqslant m$ gives,

$$\frac{d_{i+1}}{d_i} \geqslant \frac{\operatorname{ord}(D) - m}{m^2}.$$

By similar reasoning $c_{i+1}/c_i \geqslant (\operatorname{ord}(C) - i)/(i+1)^2 \geqslant 1/m^2$. It follows that when $\operatorname{ord}(D)$ is sufficiently large the sum in Eq. (12) is dominated by the latter terms, in the sense that

$$c_1 d_1 \ll c_2 d_2 \ll \cdots \ll c_{\operatorname{ord}(C)} d_{\operatorname{ord}(C)}.$$

Noting that $c_i = \sigma_{\operatorname{ord}(C)-i}(\overline{C})$, we see that $\overline{C}$ must be $\succ$-maximal. $\square$

From [5] the subpermanents $\sigma_i(A)$ for $i < 4$ are independent of the choice of $A \in \Lambda_n^k$, whereas $\sigma_4(A) = f + s(A)$ for a function f of n and k only. Hence $\succ$-maximality implies membership of S_n^k. Indeed we will see from Lemma 4 that $\succ$-maximality of $\overline{C}$ implies that both $s(C)$ and $s(\overline{C})$ are maximised. Thus Theorem 4 is concordant with (11). In general $A \succ B$ does not imply $\overline{A} \succ \overline{B}$. As an example consider $A = (I_8 + P_8 + P_8^2) \oplus (I_8 + P_8 + P_8^3)$ and $B = 2(I_8 + P_8 + P_8^4)$.

Theorem 5. *Let $k \leqslant n$ be positive integers. Every $A \in M_n^k$ is of the form*

$$A \cong aJ_k \oplus C_1 \oplus C_2 \oplus \cdots \oplus C_h$$

where $a \geqslant 0$ and $0 \leqslant h \leqslant k-1$. Moreover $G(C_i)$ is connected, $C_i \in M_{\operatorname{ord}(C_i)}^k$ and $\operatorname{ord}(C_i) \leqslant b_k^*$ *for each $i = 1, 2, \ldots, h$.*

Proof. Theorem 3 tells us that every component of $A \in M_n^k$ is of order at most b_k^*. Suppose $C_1, C_2, \ldots, C_k$ are distinct components of A. Consider the sums $s_i = \sum_{j=1}^{i} \operatorname{ord}(C_j)$. By the pigeon hole principle either there is j for which $s_j \equiv 0 \,(\mathrm{mod}\, k)$ or there are i and j for which $s_i \equiv s_j \,(\mathrm{mod}\, k)$. In either case there must be $1 \leqslant a \leqslant b \leqslant k$ for which

$\sum_{i=a}^{b} \mathrm{ord}(C_i) = lk$ for some positive integer l. Since the permanent is multiplicative on components we know each $C_i \in M^k_{\mathrm{ord}(C_i)}$ and that $C_a \oplus C_{a+1} \oplus \cdots \oplus C_b$ must achieve the maximum permanent of any matrix of its size, so $C_a \oplus C_{a+1} \oplus \cdots \oplus C_b \cong lJ_k$ by Brègman's Theorem, (1). As the above reasoning holds for any collection of k components from A, it follows that A has at most $k-1$ components which are not isomorphic to J_k. $\square$

The analogous result for permanents of the complement is:

Theorem 6. *Fix k. For sufficiently large n every* $A \in \overline{M}^k_n$ *is of the form*

$$A \cong aJ_k \oplus C_1 \oplus C_2 \oplus \cdots \oplus C_h,$$

where $a \geqslant 1$ *and* $0 \leqslant h \leqslant k-1$. *Moreover* $G(C_i)$ *is connected,* $\overline{C_i}$ *is* $\succ$*-maximal and* $\mathrm{ord}(C_i) \leqslant b^*_k$ *for each* $i = 1, 2, \ldots, h$.

Proof. The proof is along the same lines as Theorem 5. We choose n sufficiently large that Eq. (11) holds. Then for any set of k components we know that there is some subset which can be replaced by lJ_k, which uniquely maximises $s(\cdot)$ for a matrix of that size. If we also choose $n > N_{k,b^*_k}$ then each $\overline{C_i}$ must be $\succ$-maximal by Theorem 4. $\square$

We are now ready to prove a kind of periodicity in the composition of M^k_n and $\overline{M}^k_n$.

Theorem 7. *For each positive integer k there exists* η_k *such that* M^k_n *is periodic for* $n \geqslant \eta_k$ *in the sense that* $A \in M^k_n$ *if and only if* $A \oplus J_k \in M^k_{n+k}$.

Proof. If $A \oplus J_k$ maximises the permanent in Λ^k_{n+k} then any subset of the components of $A \oplus J_k$ necessarily maximises its own permanent. In particular $A \in M^k_n$. To prove the other direction, assume that $A \in M^k_n$ and $B \in M^k_{n+k}$. If $n > (k-1)b^*_k$ then Theorem 5 tells us that $B \cong J_k \oplus B'$ for some $B' \in \Lambda^k_n$. But now $\mathrm{per}(B') \leqslant \mathrm{per}(A)$ since $A \in M^k_n$ so $\mathrm{per}(B) = \mathrm{per}(B' \oplus J_k) \leqslant \mathrm{per}(A \oplus J_k)$. By our choice of B this means $\mathrm{per}(A \oplus J_k) = \mathrm{per}(B)$ and $A \oplus J_k \in M^k_{n+k}$. $\square$

Lemma 3. *If* $A, B \in \Lambda^k_n$ *and both* $\overline{A}$ *and* $\overline{B}$ *are* $\succ$*-maximal then* $\mathrm{per}(\overline{A \oplus X}) = \mathrm{per}(\overline{B \oplus X})$ *for any* $X \in \Upsilon_k$.

Proof. Since both $\overline{A}$ and $\overline{B}$ are $\succ$-maximal, we know that $\rho(\overline{A}) = \rho(\overline{B})$. By (4) it follows that $\rho(A) = \rho(B)$. The result then follows from Eq. (2). $\square$

Theorem 8. *For each positive integer k there exists* $\overline{\eta}_k$ *such that* $\overline{M}^k_n$ *is periodic for* $n \geqslant \overline{\eta}_k$ *in the sense that* $A \in \overline{M}^k_n$ *if and only if* $A \oplus J_k \in \overline{M}^k_{n+k}$.

Proof. Suppose integers n, a, k and r satisfy $n = ak + r > N_{k,\xi}$ where $0 \leqslant r < k$, $\xi = (k-1)b_k^*$ and $N_{k,\xi}$ is defined by Theorem 4. If we also suppose n is large enough to apply Theorem 6, then every $A \in \overline{M}_n^k$ can be written in the form $A \cong C \oplus lJ_k$ where l is some integer. By including some copies of J_k in our choice of C (if necessary) we can ensure that $\xi - k < \mathrm{ord}(C) \leqslant \xi$. Together with $\mathrm{ord}(C) \equiv n \bmod k$, this completely determines $\mathrm{ord}(C)$. Moreover, by Theorem 4 we know $\overline{C}$ is $\succ$-maximal. Now by applying Lemma 3 we see that the existence of a C satisfying the above conditions is both necessary and sufficient to ensure $A \in \overline{M}_n^k$. Finally, we note C depends on r but not on a. □

3. Conjectured composition of $\overline{M}_n^k$

In this section we conjecture the exact structure of matrices in S_n^k. If this structure is unique up to isomorphism and n is large then by Eq. (11) we will have identified $\overline{M}_n^k$. The basis of our conjecture is this:

Conjecture 1. Suppose $n \geqslant 2k$. If $A \in S_n^k$ then A contains J_k as a component.

If Conjecture 1 is true (which we know it is when k divides n and when n is large) then we can completely characterise S_n^k, using the following result, which must have been discovered many times.

Lemma 4. *If $A \in S_n^k$ then $\overline{A} \in S_n^{n-k}$.*

Proof. If $\overline{A} \in \Lambda_n^{n-k}$ then there are precisely k zeroes in each row and column of $\overline{A}$. Using just this information, we can count $s(\overline{A})$ by inclusion-exclusion. We do this by counting the order 2 submatrices of $\overline{A}$ according to how many zeroes they contain, yielding

$$
\begin{aligned}
s(\overline{A}) = \binom{n}{2}^2 - nk(n-1)^2 + \left[2n(n-1)\binom{k}{2} + \frac{1}{2}nk(nk-2k+1)\right] \\
- 2n\binom{k}{2}(k-1) + s(A). \qquad (13)
\end{aligned}
$$

This shows that $s(\overline{A}) - s(A)$ is a function of n and k only and does not depend on the structure of A. □

Armed with Conjecture 1 and Lemma 4 we can inductively find the matrices in S_n^k. If $n \geqslant 2k$ we can strip off a copy of J_k and otherwise we consider the complementary case S_n^{n-k} and note that $n < 2k \Rightarrow n > 2(n-k)$. This process yields the following corollary of Conjecture 1:

Conjecture 2. Let q_i and r_i be the quotients and remainders derived by applying the division algorithm to n/k. Specifically, we define $r_0=n$ and $r_1=k$ and then proceed inductively using $0 \leqslant r_{i+1}=r_{i-1}-q_i r_i<r_i$ until a zero remainder is found. Let r_z be the last non-zero remainder. If $A \in S_n^k$ then

$$A \cong (q_1-1)J_{r_1} \oplus \overline{q_2 J_{r_2} \oplus \overline{q_3 J_{r_3} \oplus \cdots \oplus \overline{q_{z-1} J_{r_{z-1}} \oplus \overline{(q_z+1)J_{r_z}}}}}. \tag{14}$$

Let $\{b_i\}_i$ be the block sizes in (14) arranged in non-increasing order. That is, let $b_1=b_2=\cdots=b_{q_1-1}=r_1$ and $b_{q_1}=b_{q_1+1}=\cdots=b_{q_1+q_2-1}=r_2$ etc. A simple consequence of Conjecture 2 would be:

Conjecture 3. If $A \in \Lambda_n^k$ then

$$s(A) \leqslant \binom{k}{2} \sum_i \binom{b_i}{2} + \sum_{i<j} \binom{k-b_i}{2} b_i b_j$$

with equality if and only if A satisfies (14).

Our next result shows that Conjecture 2 implies a distinction between M_n^k and $\overline{M}_n^k$ in many cases.

Theorem 9. *Let $d \geqslant 2$ be fixed. For t sufficiently large,* $\operatorname{per}(dD_{t+1})>\operatorname{per}((d-1)J_t \oplus X)$ *regardless of the choice of $X \in \Lambda_{t+d}^t$.*

Proof. We use two particular instances of (5):

$$\operatorname{per}(D_{t+1})=(t+1)!\left(1-\frac{1}{t+1}\right)^{t+1} \exp\left(\frac{1}{2(t+1)}+\frac{1}{3(t+1)^2}+\mathrm{O}(t^{-3})\right)$$

and

$$\operatorname{per}(X)=(t+d)!\left(1-\frac{d}{t+d}\right)^{t+d} \exp\left(\frac{d}{2(t+d)}+\frac{d(3d-1)}{6(t+d)^2}+\mathrm{O}(t^{-3})\right)$$

for $X \in \Lambda_{t+d}^t$. Now applying 6.1.47 of [1] for $t \to \infty$, gives

$$\frac{(t+1)!^d}{t!^{d-1}(t+d)!}=1-\frac{d(d-1)}{2(t+1)}+\frac{d(d+1)(d-1)(3d-2)}{24(t+1)^2}+\mathrm{O}(t^{-3}).$$

Combining the above results yields

$$\frac{\operatorname{per}(D_{t+1})^d}{\operatorname{per}(J_t)^{d-1}\operatorname{per}(X)}=1+\frac{d(d-1)}{4t^2}+\mathrm{O}(t^{-3})$$

from which the result follows. $\square$

Note that Conjecture 2 implies that matrices in $\overline{M}_n^k$ are constructed by taking the maximum possible number of copies of J_k, together with a single component which uses the remainder of the space. However, Theorem 9 shows this approach does not (always) work for constructing matrices in M_n^k.

Further evidence for a distinction in general between M_n^k and $\overline{M}_n^k$ is provided by considering an arbitrary $X \in \Lambda_{k+2}^k$ for some $k > 1$. By (13),

$$s(J_k \oplus X) - s(2D_{k+1}) = k - 1 + s(\overline{X}) - 2s(I_{k+1}) \geqslant k - 1 > 0, \tag{15}$$

which demonstrates that no matrix in S_n^k can contain more than one copy of D_{k+1}. Of course, for large n the same is true for elements of $\overline{M}_n^k$ by (11).

Suppose $n = tk - r$ for $0 < r \leqslant k$ and $t > k - r$. Let $A \in \Lambda_n^k$ be defined by (14) and let $B \cong (t - k + r - 1)J_k \oplus (k - r)D_{k+1}$. For $k \geqslant 5$ Merriell [7] conjectured that $A \in M_n^k$ when $r = 1$ and that $B \in M_n^k$ when $r \geqslant 3$. Some known counterexamples to this conjecture are discussed is [6]. For moderate values of n and k it is easy to compare per(A) to per(B) using Eq. (2). Such a computation suggests that

$$\mathrm{per}(A) > \mathrm{per}(B) \text{ for } \begin{cases} k \geqslant 3r + 2 & \text{when } r = 1, 2, \\ k \geqslant 3r + 1 & \text{when } r = 3, 4, \ldots, 39, \\ k \geqslant 3r & \text{when } r = 40, 41, \ldots, 50, \end{cases} \tag{16}$$

whereas per(A) < per(B) otherwise (provided $r \leqslant 50$). In particular, Eq. (16) provides a wealth of counterexamples to Merriell's conjecture when $r > 2$ and $k > 3r$, the smallest being $A = 6J_{10} \oplus J_7 \oplus \overline{2J_3 \oplus D_4} \in \Lambda_{77}^{10}$. By contrast Theorem 9 provides strong evidence to support the conjecture when $k - r \ll k$.

4. Some examples

We examine the relationship between M_n^k and $\overline{M}_n^k$ for some particular values of k. The smallest case of interest is $k = 2$. Here it is known (e.g. [3,6]) that $M_n^k = \overline{M}_n^k$ for $n = 2, 3, 4$ and for $n \geqslant 8$.

We look next at the $k = 3$ case. It follows from (1) and [6] that $\overline{M}_{3t}^3 = M_{3t}^3$ for all integers $t \geqslant 4$. So consider the cases $n = 3t + 1$ and $n = 3t + 2$. Merriell [7] showed for $r = 1, 2$ and $t \geqslant r$ that M_{3t+r}^3 consists of precisely those A for which $A \cong rD_4 \oplus (t - r)J_3$. The one unusual case is M_5^3 which consists of $\overline{I_5 + P_5}$ and its permutations. Clearly, if we choose n large then $M_{3t+2}^3 \cap \overline{M}_{3t+2}^3 = \emptyset$ by (15).

In fact it is not hard to establish Conjecture 1 for $k = 3$ (it is trivial for $k < 3$). Suppose $A \in S_n^3$ for $n > 6$ and A does not contain J_3 as a component. Let K be the graph $K_{3,3}$ with one edge removed. Then $G(A)$ cannot contain K as an induced subgraph; if it did then an edge switching argument could increase $s(A)$. Since $G(A)$ contains no copies of $K_{3,3}$ or K, the number of 4-cycles incident with a vertex never exceeds 3, so $s(A) \leqslant 3n/2$. Now observe that

$$\begin{aligned} &s(D_4 \oplus (t - 1)J_3) = 3n - 6, \\ &s(\overline{J_2 \oplus D_3} \oplus (t - 1)J_3) = 3n - 9 \end{aligned} \tag{17}$$

and in either case these values exceed $s(A)$. This is sufficient to prove Conjecture 1 for $k=3$, namely that the matrices shown in (17) (and their permutations) constitute $\overline{M}_n^3$ for large n not divisible by 3. The evidence in [6] suggests that 'large' in this context may mean $n \geqslant 10$.

Next we conjecture the answers for $k=4$ and 5. By developing the arguments of the previous case, it is possible to find S_n^4. However, to determine M_n^4 we need to assume a specific bound on component size, say $b_4^* \leqslant 9$. Under this assumption, when t is large:

$$M_{4t}^4 = \overline{M}_{4t}^4 = \{A \cong tJ_4\},$$

$$M_{4t+1}^4 = \overline{M}_{4t+1}^4 = \{A \cong D_5 \oplus (t-1)J_4\},$$

$$M_{4t+2}^4 = \{A \cong \overline{2D_3} \oplus (t-1)J_4\}, \quad \overline{M}_{4t+2}^4 = \{A \cong \overline{3J_2} \oplus (t-1)J_4\},$$

$$M_{4t+3}^4 = \{A \cong \overline{2D_3} \oplus D_5 \oplus (t-2)J_4\}, \quad \overline{M}_{4t+3}^4 = \{A \cong \overline{J_3 \oplus D_4} \oplus (t-1)J_4\}.$$

Known exceptions to the above rules for small n are M_7^4, $\overline{M}_9^4$, $\overline{M}_{10}^4$ and $\overline{M}_{11}^4$. From [6] there are no other exceptions for $n < 17$ unless $b_4^* > 11$.

Similarly we handle the $k=5$ case by assuming $b_5^* \leqslant 9$. Then for large t,

$$M_{5t}^5 = \overline{M}_{5t}^5 = \{A \cong tJ_5\},$$

$$M_{5t+1}^5 = \overline{M}_{5t+1}^5 = \{A \cong D_6 \oplus (t-1)J_5\},$$

$$M_{5t+2}^5 = \{A \cong 2D_6 \oplus (t-2)J_5\}, \quad \overline{M}_{5t+2}^5 = \{A \cong \overline{2J_2 \oplus D_3} \oplus (t-1)J_5\},$$

$$M_{5t+3}^5 = \{A \cong \overline{2D_4} \oplus (t-1)J_5\}, \quad \overline{M}_{5t+3}^5 = \{A \cong \overline{J_3 \oplus \overline{J_2 \oplus D_3}} \oplus (t-1)J_5\},$$

$$M_{5t+4}^5 = \{A \cong Q \oplus (t-1)J_5\}, \quad \overline{M}_{5t+4}^5 = \{A \cong \overline{J_4 \oplus D_5} \oplus (t-1)J_5\},$$

where

$$Q = \begin{pmatrix} 1&1&1&1&1&0&0&0&0 \\ 1&1&1&1&1&0&0&0&0 \\ 1&1&1&1&0&0&1&0&0 \\ 1&1&1&1&0&1&0&0&0 \\ 1&1&0&0&1&0&0&1&1 \\ 0&0&0&1&0&1&1&1&1 \\ 0&0&1&0&0&1&1&1&1 \\ 0&0&0&0&1&1&1&1&1 \\ 0&0&0&0&1&1&1&1&1 \end{pmatrix}.$$

The exceptions in [6] are M_7^5, $\overline{M}_8^5$, $\overline{M}_{12}^5$, $\overline{M}_{13}^5$ and $\overline{M}_{14}^5$.

5. Consequences

The characterisations in Theorems 5 and 6 show that elements of the sets M_n^k and $\overline{M}_n^k$ are similar (although Theorem 9 pointed to a likely distinction). That both sets exhibit a kind of periodicity in n was demonstrated by Theorems 7 and 8.

All our results help to answer problem 4 of [8], which asks for the maximum permanent in Λ_n^k, in the case when k does not divide n. We have also partly answered problem 12 from the same source. Let $\Delta_n^k \subset \Lambda_n^k$ denote the set of all circulant matrices in Λ_n^k; that is the matrices which are sums of powers of P_n. Minc's problem 12 asks, in part, whether there exists a matrix in Λ_n^k whose permanent strictly exceeds the permanent of every circulant in Δ_n^k. Note that the number of rows of a circulant which are equal to a given row does not depend on which row is chosen. Hence, if $C \in \Delta_n^k$ contains J_k as a component, then k divides n and $C \cong (n/k)J_k$. Thus by Theorem 5 we see that M_n^k and Δ_n^k are disjoint provided $n \not\equiv 0 \bmod k$ is large enough. Finally, we observe that a matrix is a circulant if and only if its complement is a circulant, and that $\overline{M}_n^k$ and Δ_n^k are also disjoint for large $n \not\equiv 0 \bmod k$, by Theorem 6. In other words the answer to Minc's problem 12 is that the maximum permanent in Λ_n^k is generally not achieved by a circulant. The cases when k divides n or $(n-k)$ divides n are thus exceptional in this regard, [6].

We also draw attention to the ramifications of Conjecture 2 for the four part research problem given in [6]. If true it would confirm that when n is large enough $A \in \overline{M}_n^k$

(a) is unique up to isomorphism,

(b) contains the maximum possible number of components and

(d) can be constructed up to isomorphism, using only zero matrices, complementation and the direct sum operator.

However the third part [(c) that $A \in M_n^k$] would often fail, according to Theorem 9. Note that if Conjecture 2 turns out to be false then Lemma 3 leaves open the possibility of (a) failing. Also, Theorem 3 represents a proof of a weakened form of (b).

Our final comment pertains to the opposite problem to the one we have dealt with. Although Schrijver [9] recently proved a nice lower bound on the permanent in Λ_n^k, little is known about the matrices which achieve the minimum value. Such questions are beyond the scope of this paper. However, some day it may be possible to shed light on them by employing some of the same techniques we have used for the maximising problem.

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